New Triplet State Organic Ions

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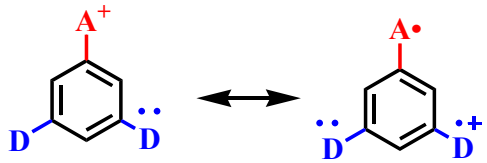
Paramagnetic organic molecules such as free radicals, carbenes, etc. are interesting because of the potential for creating new materials with interesting bulk magnetic properties. Computational studies done in Falvey and Cramer's labs have identified a a new class of organic species that have paramagnetic or triplet ground states. These consist of benzene ring having one or two electron donor groups substituted meta to a strong electron acceptor. Example of this class of triplet molecules includes nitrenium ions, carbenium ions, and oxenium ions. Analysis of the electron distributions from these calculations shows that these meta donor-acceptor ions are analogous to the well known non-Kekule diradical, meta-xylylene.



Examples predicted to be ground state triplets